

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol  
647-42-7 | DTXSID5044572

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.91 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Butene, 1,1,1,2,3,4,4,4-octafluoro-</div> <div>Measured: 1.33e-01</div> <div>Predicted: 2800</div>	<div>Image not found</div> <div>1,2-Dichloro-4-(trifluoromethyl)benzene</div> <div>Measured: 5.25e-01</div> <div>Predicted: 2.42</div>	<div>Image not found</div> <div>Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-</div> <div>Measured: 33.1</div> <div>Predicted: 2170</div>
<div>Image not found</div> <div>1-Decene</div> <div>Measured: 159</div> <div>Predicted: 1.31</div>	<div>Image not found</div> <div>Ethylene sulfide</div> <div>Measured: 46.1</div> <div>Predicted: 166</div>	